

CLAIMS

What is claimed is:

1. An instrument comprising:
an ionization source configured to apply different ionization energies to a sample to provide different sample characteristics; and
processing circuitry configured to process the different sample characteristics to
5 identify the sample.
2. The instrument of claim 1 wherein the ionization source comprises an electron impact ionization source and one of the ionization energies comprises 70 eV.
3. The instrument of claim 1 wherein at least one of the sample characteristics comprises mass spectra of the sample.
- 10 4. The instrument of claim 1 wherein the process circuitry is configured to acquire at least two data sets of the different sample characteristics, one of the two data sets of the different sample characteristics comprising a first sample characteristic associated with a first ionization energy and another of the two data sets of the different sample characteristics comprising a second sample characteristic associated with a
15 second ionization energy.
5. The instrument of claim 4 wherein the processing circuitry is further configured to access at least two data sets of reference sample characteristics, one of the data sets of the reference sample characteristics comprising a third reference sample characteristic associated with the first ionization energy and another of the two data sets of
20 the reference sample characteristics comprising a fourth reference sample characteristic associated with the second ionization energy.
6. The instrument of claim 5 wherein the processing circuitry is further configured to compare the data sets of the different sample characteristics with the data sets of the reference sample characteristics and calculate a match value.

7. A mass spectrometer comprising:

an ionization component configured to receive a sample and provide a first ionization energy to the sample to form a first ionized analyte and provide a second ionization energy to the sample to form a second ionized analyte, wherein the first and

5 second energies are not equal;

a detection component configured to detect the first and second ionized analytes formed by the ionization component; and

processing circuitry configured to monitor the detection component and associate detection of the first ionized analytes with a first sample characteristic and associate
10 detection of the second ionized analytes with a second sample characteristic, wherein the processing circuitry is further configured to associate both the first sample characteristic with the first ionization energy, and the second sample characteristic with the second ionization energy to identify a sample.

8. The mass spectrometer of claim 7 wherein the sample characteristics

15 comprise mass spectra and the processing circuitry is further configured to prepare a sample data set comprising first and second data sets, the first data set comprising the first mass spectra associated with the first ionization energy and the second data set comprising second mass spectra associated with the second ionization energy.

9. The mass spectrometer of claim 8 further comprising storage circuitry

20 comprising media configured to store digital data, wherein the media comprises reference data comprising third and fourth data sets, the third data set comprising a third mass spectra and the first ionization energy and the fourth data set comprising a fourth mass spectra and the second ionization energy, wherein the third mass spectra was acquired at the first ionization energy and the fourth mass spectra was acquired at the second
25 ionization energy.

10. The mass spectrometer of claim 9 wherein the processing circuitry is

further configured to compare the sample and reference data, the comparing comprising applying an algorithm to both the mass spectra of the first data set and the third data set, and the mass spectra of the second data set and the fourth data set, the algorithm
30 configured to compare mass spectra and provide a first match value of the mass spectra of the first data set and the mass spectra of the third data set and a second match value of the mass spectra of the second data set and the mass spectra of the fourth data set.

11. The mass spectrometer of claim 10 wherein the processing circuitry is further configured to provide an average of the first match value and the second match value.

12. The mass spectrometer of claim 7 wherein the first ionization energy
5 comprises electron impact ionization energy of about 10 eV and the second ionization energy comprises electron impact ionization energy of about 70 eV.

13. The mass spectrometer of claim 7 wherein the ionization component comprises first and second ionization sources, the first ionization source being configured to provide the first ionization energy and the second ionization source being configured to
10 provide the second ionization energy, wherein the first ionization parameter comprises electron impact ionization energy and the second ionization energy comprises chemical ionization energy.

14. The mass spectrometer of claim 7 wherein:
the ionization component is further configured to provide the first ionization energy
15 to the sample at a first moment in time and the second ionization energy to the sample at a second moment in time; and

the processing circuitry is configured to correlate both the first ionization energy provided with the first ionized analytes detected during the first moment in time, and the second ionization energy provided with the second ionized analytes detected during the
20 second moment in time.

15. The mass spectrometer of claim 7 further comprising:
storage circuitry comprising a plurality of data sets, each of the data sets comprising a reference sample characteristic associated with one of the first or second ionization energies; and
25 wherein the processing circuitry component is further configured to access the data sets responsive to the detection of the first and second ionized analytes and determine a match value.

16. The mass spectrometer of claim 7 further comprising:

a mass separation component configured to receive the first and second ionized analytes from the ionization component and provide a first separation waveform to

separate a first mass-to-charge ratio range of ionized analytes and provide a second

5 separation waveform to separate a second mass-to-charge ratio range of ionized analytes; and

wherein the processing circuitry is further configured to associate both the first sample characteristic with the first mass separation waveform, and the second sample characteristic with the second mass separation waveform.

10 17. The mass spectrometer of claim 16 wherein the ionization component comprises an electron impact ion source component and the first ionization energy comprises an electron impact energy of about 10 eV and the second ionization energy comprises an electron impact energy of about 70 eV.

15 18. The mass spectrometer of claim 16 wherein the ionization component comprises an electron impact ion source and the mass separator component comprises an ion trap.

19. The mass spectrometer of claim 16 wherein the processing circuitry is further configured to prepare a sample data set comprising first and second data sets, the first data set comprising the first sample characteristics associated with the first ionization
20 energy and mass separation waveforms and the second data set comprising the second sample characteristic associated with the second ionization energies and mass separation waveforms.

20. The mass spectrometer of claim 16 further comprising storage circuitry comprising media configured to store the sample data set and a reference data set, the
25 reference data set comprising third and fourth data sets, the third data set comprising a third sample characteristic of a reference sample associated with the first ionization energy and mass separation waveforms and the fourth data set comprising a fourth sample characteristic of the reference sample associated with the second ionization energy and mass separation waveforms, wherein the third sample characteristic was acquired utilizing
30 the first ionization energy and mass separation waveforms and the fourth sample characteristic was acquired utilizing the second ionization energy and mass separation waveforms.

21. The mass spectrometer of claim 20 wherein the mass separation waveforms are not equal.

22. A mass spectrometer of comprising:

a first analyte modification component configured to receive a sample and provide
5 both a first ionization energy to the sample to form a first group of ionized analytes, and provide a second ionization energy to the sample to form a second group of ionized analytes;

a first mass separation component configured to receive the first and second groups of ionized analytes and provide both a first separation waveform to separate a first
10 mass-to-charge ratio range of the first group of ionized analytes, and provide a second separation waveform to separate a second mass-to-charge ratio range of the second group of ionized analytes;

a second analyte modification component configured to receive the first and second mass-to-charge ratio ranges of ionized analytes and provide both a third energy to
15 the first and second ranges of ionized analytes to form a third group of ionized analytes, and provide a fourth energy to the ranges to form a fourth group of ionized analytes;

a second mass separation component configured to receive the third and fourth groups of ionized analytes and provide both a third separation waveform to separate a third mass-to-charge ratio range of the third group of ionized analytes and provide a fourth
20 separation waveform to separate a fourth mass-to-charge ratio range of the fourth group of ionized analytes, wherein at least one of the first and second or third and fourth ionization energies, or the first and second or third and fourth separation waveforms are not equal;

a detection component configured to detect the ionized analytes of the third and fourth ranges of ionized analytes received from the second mass separation component;
25 and

processing circuitry configured to monitor the detection component and associate detection of ionized analytes of the third range with a first sample characteristic and associate detection of ionized analytes of the fourth range with a second sample characteristic, wherein the processing circuitry is further configured to correlate both the
30 first sample characteristic with one or more of the first ionization energy, the first mass separation waveform, the third energy and the third mass separation waveform, and the second sample characteristic with one or more of the second ionization energy, the second mass separation waveform, fourth ionization energy, and the fourth separation waveform.

23. The mass spectrometer of claim 22 wherein both the first and second analyte modification components comprise electron impact ionization sources and the ionization energy of the first source of the first data set comprises about 10 eV and the ionization energy of the first source of the second data set comprises about 70 eV.

5 24. The mass spectrometer of claim 23 wherein the second analyte modification component comprises a collisionally induced dissociation source and the third and fourth energies comprise collisionally induced dissociation energies.

25. The mass spectrometer of claim 22 wherein both the first and second mass separation components comprise ion traps.

10 26. The mass spectrometer of claim 25 wherein the second ion trap is configured to isolate individual analytes of a predefined mass-to-charge ratio.

27. An article of manufacture comprising:
media comprising digital data usable for identifying samples, the digital data comprising:

15 a first set of data comprising a plurality of mass spectrometry reference sample characteristics associated with a first mass spectrometry acquisition parameter; and

a second set of data comprising a plurality of mass spectrometry reference sample characteristics associated with a second mass spectrometry acquisition parameter, wherein individual ones of the sample characteristics of the first set are associated with individual ones of the sample characteristics of the second set; and
20 wherein the first and second sets of data may be accessed and utilized to identify a sample.

25 28. The article of claim 27 wherein the mass spectrometry reference sample characteristics comprise mass spectra.

29. The article of claim 27 wherein the first and second sets of data are configured to be accessed responsive to a plurality of analytes generated using a plurality of mass spectrometry acquisition parameters.

30 30. The article of claim 27 wherein at least one of the plurality of acquisition parameters comprises a parameter of an ionization component.

31. The article of claim 30 wherein the ionization component parameter comprises ion source energy.

32. The article of claim 31 wherein the ion source energy of the first data set is less than the ion source energy of the second data set.

5 33. The article of claim 27 wherein the individual ones of the sample characteristics of the first and second sets of data are each associated with a plurality of mass spectrometry acquisition parameter values.

34. The article of claim 33 wherein the acquisition parameters further comprise a parameter of a mass separation component.

10 35. The article of claim 34 wherein the mass separation component parameter comprises a mass separation waveform.

36. A sample analysis method comprising:
providing a sample;

generating a sample data set using the sample, the sample data set comprising
15 first and second data sets, wherein each of the first and second data sets comprises at least one of an analytical parameter value and a sample characteristic acquired using the analytical parameter value, wherein the analytical parameter value of the first set is different than the analytical parameter value of the second set; and
using the first and the second data sets, identifying the sample.

20 37. The analysis method of claim 36 wherein the generating comprises:
generating a plurality of analytes; and
detecting the analytes to generate a plurality of spectra, wherein the sample characteristics comprise the spectra.

38. The analysis method of claim 36 wherein the analytical parameter value a
25 parameter value of one or more of a sample inlet component, an analyte modification component, a mass separation component, and a detection component..

39. The analysis method of claim 38 wherein the analyte modification parameter value comprises an ionization energy applied by an ionization source.

40. The analysis method of claim 39 wherein the analyte modification parameter value of the first data set comprises a first ionization energy and the analyte modification parameter value of the second data set comprises a second ionization energy, wherein the value the first ionization energy is lower than the second ionization
5 energy.

41. The analysis method of claim 36 wherein the analytical parameter value comprises a parameter value of one or more of a sample inlet component, an analyte modification component, a mass separation component, and a detection component and the generating the sample data set comprises:
10 generating a first plurality of ionized analytes at a first analyte modification parameter value;
separating a first group of the ionized analytes from the plurality at a first mass separation parameter value; and
generating a second plurality of ionized analytes from the first group of ionized
15 analytes at a second analyte modification parameter value; and
separating a second group of ionized analytes from the second plurality at a second mass separation parameter value, the sample characteristic comprising the spectra of the second group of ionized analytes , wherein the first and second data sets comprise one or more of the first and second analyte modification and mass separation
20 parameter values.

42. The analysis method of claim 41 wherein the first and second mass separation parameters are the same.

43. The analysis method of claim 42 wherein the first mass separation parameter value of the first data set does not equal the first mass separation parameter
25 value of the second data set.

44. The analysis method of claim 41 wherein the mass separation parameter value of the first and second data sets comprises a mass range value.

45. The analysis method of claim 44 wherein the first analyte modification parameter value of the first set does not equal the first mass separation parameter value of
30 the second data set.

46. The analysis method of claim 45 wherein the first analyte modification parameter value of the first and second data sets comprises and ion source energy.

47. The analysis method of claim 41 wherein the first and second mass separation parameters are different.

48. The analysis method of claim 47 wherein the first mass separation parameter value comprises a predefined mass-to-charge ratio isolation value and the
5 second mass separation parameter value comprises a mass-to-charge range.

49. The analysis method of claim 48 wherein the predefined mass-to-charge ratio isolation value of the first set of data does not equal the predefined mass-to-charge ratio isolation value of the second set of data.

50. The analysis method of claim 41 wherein the identifying the sample
10 comprises:
providing a reference data set comprising the sample characteristics of a reference sample and one or more of the first analyte modification parameter value, the second analyte modification parameter value, the first mass separation parameter value, and the second mass separation parameter value; and
15 comparing the reference data set to the sample data set.

51. The mass analysis method of claim 36 wherein the sample characteristic comprises at least mass spectra and the identifying the sample further comprises:
providing a reference data set comprising third and fourth data sets, the third data set comprising the analytical parameter value of the first set and mass spectra of a
20 reference sample generated using the analytical parameter value of the first set, and the fourth data set comprising the analytical parameter value of the second set and mass spectra of the reference sample generated using the analytical parameter value of the second set; and
comparing the sample and reference data sets, the comparing comprising applying
25 an algorithm to both the mass spectra of the first data set and the third data set, and the mass spectra of the second data set and the fourth data set, wherein the algorithm is configured to compare mass spectra and provide a first match value of the mass spectra of the first data set and the mass spectra of the third data set and a second match value of the mass spectra of the second data set and the mass spectra of the fourth data set